IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_VOC13

This data sheet updated: 12th December 2007 (with no revision of the preferred values).

$O_3 + CH_2=C(CH_3)C(O)OONO_2$ (MPAN) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate Coefficients			
$(8.2 \pm 2.0) \times 10^{-18}$	295 ± 5	Grosjean et al., 1993	(a)

Comments

(a) Experiments were carried out at atmospheric pressure of air, by monitoring the decay rates of $CH_2=C(CH_3)C(O)OONO_2$ (MPAN) in the presence of known excess concentrations of O_3. Cyclohexane was added to the reactant mixtures to scavenge any OH radicals present. MPAN concentrations were measured by GC with electron capture detection.

Preferred Values

$k = 8.2 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.3$ at 298 K.

Comments on Preferred Values

The preferred value is based on the sole study of this reaction by Grosjean et al. (1993). The rate coefficient for this reaction is similar in magnitude to those for the reactions of O_3 with propene (Atkinson, 1997; IUPAC, 2007) and 2-methylpropene (Atkinson, 1997), and a factor of 5 higher than that for the reaction of O_3 with ethane (Atkinson, 1993; IUPAC, 2007). This reactivity of MPAN towards O_3 is consistent with the recommended rate coefficient for the reaction of MPAN with HO radicals (IUPAC, 2007). The reaction of O_3 with MPAN proceeds by initial addition of O_3 to the C=C bond, and formaldehyde has been observed as a reaction product with a formation yield of 60 ± 10% (Grosjean et al., 1993).

References

Atkinson, R.: J. Phys. Chem. Ref. Data, 26, 215, 1997.
Grosjean, D., Grosjean, E. and Williams II, E. L.: Environ. Sci. Technol., 27, 2548, 1993.
IUPAC,: http://iupac.pole-ether.fr, 2013.